Open Journal of Physical Chemistry, 2011, 1, 61-69
doi:10.4236/ojpc.2011.13009 Published Online November 2011 (http://www.SciRP.org/journal/ojpc)

Data Consistency Tests through the Use of Neural Networks and Virial Equation. Application of the Proposed Methodology to Critical Study of Density Data

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Received May 30, 2011; *revised August* 9, 2011; *accepted September* 11, 2011

Abstract

This paper focuses on a very important point which consists in evaluating experimental data prior to their use for chemical process designs. Hexafluoropropylene *P*, ρ, *T* data measured at 11 temperatures from 263 to 362 K and at pressures up to 10 MPa have been examined through a consistency test presented herein and based on the use of a methodology implying both neural networks and Virial equation. Such a methodology appears as very powerful to identify erroneous data and could be conveniently handled for quick checks of databases previously to modeling through classical thermodynamic models and equations of state. As an application to liquid and vapor phase densities of hexafluoropropylene, a more reliable database is provided after removing out layer data.

Keywords: Consistency Tests, Hexafluoropropylene, Neural Networks, Vibrating Tube Densimeter, Virial Equation

1. Introduction

Nowadays a great concern towards the environment protection is shown by the refrigeration industry which is urged to find new fluids as refrigerants substitutes. In Montreal Protocol (1987) it was decided to phase out and replace ozone-depleting refrigerants like chlorofluorocarbons (CFC's) and hydrochlorofluorocarbons (HCFC's). Consequently CFCs were prohibited in 1996 by the signing of Montreal Protocol countries and the fixed deadline for a total banishment of HCFC's which have low ozone depletion potential was set , *i.e.* 2030 [1].

Alternative compounds must be found and hexafluoropropene (HFP, R1216), CAS Number 116-15-4 is good candidate with its 0.86 GWP value [2], eventually mixed to other components. Numerous data concerning volumetric properties of this compound obtained using the vibrating-tube densitometer technique are available in Coquelet *et al.* paper [3]. They correspond to *P*, ρ, *T* triplets belonging to 11 isotherms reported partly in tables 2 and 3. It is highly recommended prior to using data for process design to have serious estimation about their reliability and their accuracy, mainly in order not to take too big error margins. The best recommendation that could be done to experimental laboratories would be the use of several experimental techniques to check for reproducibility of data [4] and consequently provide guaranteed data. Young researchers must be encouraged to handle experimental works that are so useful to industry and theoricists [5]. Collaborations between laboratories with complementary skills in either experimental, modeling and simulation are a real advantage for presenting worth and reliable data. Starting a French thermodynamic research federation under the auspices of CNRS is in project along with the setup of an international network. The following sentence [6]: "All of the just mentioned points need to be addressed in the frame of a thermodynamicists' network. This is one of the urgent goals to be achieved in the near future" is found just after a list of comments and remarks done during round table discussions.

For low pressure *PVT* data, a very simple test consists in verifying the data do follow the virial equation and agree with the perfect gas law when pressure tends to

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zero (density tends to zero while pressure tends to zero).

For high pressure *PVT* data, the use of a flexible model, as a neural network based model, allows testing internal constancy of data.

These approaches are enlightened in this paper. They are complementary tests to over, for example see references [7-9], but are the most convenient here, in the considered pressure range.

2. Thermodynamic Consistency of Data in Vapor Phase through the Virial Equation

At low pressures the use of the virial equation is quite convenient to check for data consistency with respect to vapor phase. Indeed, it is well known that the virial equation, truncated after the 3rd term allows acceptable representation of *PVT* data of pure compounds at low and medium pressures (up to about 2 MPa).

This equation is written as:

$$P.v/R.T = 1 + B/v + C/v^2 \tag{1}$$

with B and C being the 2nd and 3rd virial coefficients.

These two parameters can be adjusted from isothermal experimental data by rewriting Equation (1) as:

$$(P.v/R.T\text{-}1\ ).\ v = B + C/v \tag{2}$$

By tracing the evolution of the $((P.v/R.T)\text{-}1).\ v$ term versus $1/v$, it is possible to check for the linearity of Equation (2). Applied to data at 348.1 K, the results are shown in **Figure 1**. Perfect linearity is observed for 1 / v above 0.4 $kmol{\cdot}m^{-3}$ *i.e.* above 1.0 MPa. But, at lower pressures, the experimental points depart significantly from linearity. Experimental uncertainties cannot explain these discrepancies while the virial equation is all the more justified for the lowest pressures.

Such departures, at low pressures, displayed at 348.1 K are observed for all of the other temperatures. This observation proves that although the densimeter vibrating tube [3] is ideal for measuring medium or high density values it is no longer the ideal tool for very low densities.

Although a low pressure "pressure transducer" was used, when working at the lowest pressures, this was not the solution for ensuring quality density values. It is reasonable to believe that densimeter designed for working at pressures up to 40 MPa, is not convenient at low pressures because of its thick-walled (not sensitive enough) vibrating tube.

For low pressures, the values of data P.V.T can be extrapolated preferably and conveniently from the data obtained at higher pressures, by using the virial equation. In **Table 1**, are given the values of the 2nd and 3rd virial coefficients calculated from the reliable part of the data.

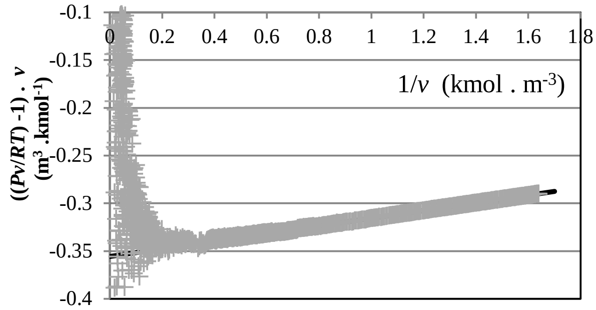

Figure 1. Data departure from virial equation at 348.1 K.

Table 1. 2nd and 3rd virial coefficients as a function of temperature.

T	B	C
K	$m^3{\cdot}kmol^{-1}$	$m^6{\cdot}kmol^{-2}$
283.24	–0.5400	–0.17000
303.28	–0.4880	–0.01124
323.21	–0.4283	0.04116
343.26	–0.3720	0.04303
348.12	–0.3556	0.04015
353.12	–0.3432	0.03953
355.27	–0.3384	0.03920
357.06	–0.3344	0.03912
358.16	–0.3325	0.03903
362.90	–0.3201	0.03743

3. Thermodynamic Consistency of Data in Liquid Phase through a Multiparameter Model

A multiparameter model allows the representation of experimental data within their experimental uncertainties, provided the uses of a sufficient number of parameters and the availability of great enough number of data.

When a reduced number of data are not consistent with respect to main part of database, the model will lead to a representation presenting deviations much higher than estimated values of experimental uncertainties. Consequently, doubtful data will be easily identified through deviation plots.

Multiparameter models must have certain characteristics: they must be very flexible and able to admit a great number of parameters. A neural network based model has all these characteristics. It will be used in this work. Detailed description of neural network models is given elsewhere [10,11]. **Figure 2** shows the topology of a neural network with only one hidden layer. The activation function, used herein, is the sigmoid one. Through optimization procedure the adequate number of neurons in hidden layer was found to be 7, allowing both under and over-fittings. The two neurons in the input layer represent the following independent variables: temperature T and density ρ, while the output variable is the pressure P. All variables are normalized between 0.1 and 0.9 to deal with

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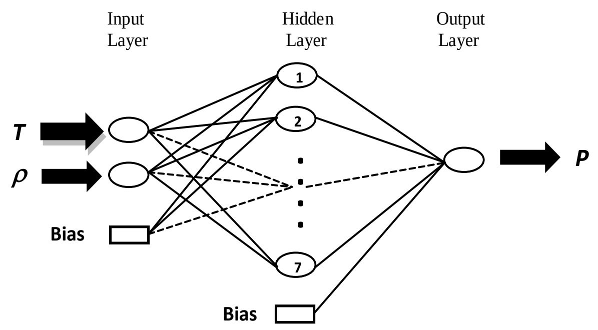

Figure 2. Neural network topology.

large variable ranges.

We have selected 4300 triplets in a random way among not the published data 3 but the raw data as they were got by the authors through their data acquisition unit (about 48,000 (P, ρ, T) triplets), for the training the network (adjustment of its 29 parameters). This permits observing the deviations between experimental and calculated pressures for these 48,000 triplets. It is worth to use raw data instead of published data as they are not rounded and consequently have more digits available for mathematical treatments. Special behavior is pointed out at 348.2 K, see **Figure 3**. In fact, between 8.5 and 10 MPa, several points evolve in a way different from most of the others. To enlight clearly this problem, we have plotted (see **Figure 4**) the density as a function of pressure in the (8-10) MPa range. One observes two distinct series of data. The series corresponding to the lowest density values but also to the highest Pexp-Pcal deviations must be eliminated from the corresponding isothermal set data (30 experimental points). A new neural network treatment on the 348 K isothermal data after removing doubtful data was carried out adjusting again 29 parameters. Even after discarding these 30 experimental points too high deviations are still observed; they concern 450 data that must be also discarded. Four successive treatments have been necessary to obtain a clean coherent dataset (deviations in agreement with estimated experimental uncertainties).

Behaviors similar to those displayed in **Figures 3** and **4** are found at all temperatures. Corresponding complementary figures are available upon request to the corresponding author of this paper. All isothermal data at 355.2 K must be rejected, the reason of rejection being the high standard deviation that is observed between experimental and calculated pressures; It is, in fact, 5 times bigger for this isotherm than for all other isotherms. Finally, 42,240 triplets are considered as trustable over the 48,000. Pressure deviations corresponding to these 42,240 triplets are plotted in **Figure 5**. They are contained in +/– 0.04 MPa pressure range, although authors [3] claimed for pressure uncertainties within 0.0003 or 0.0006 MPa, depending on

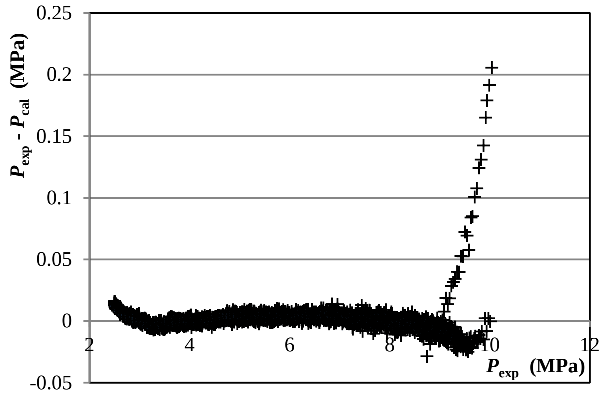

Figure 3. Deviations between experimental and calculated pressures at 348.2 K.

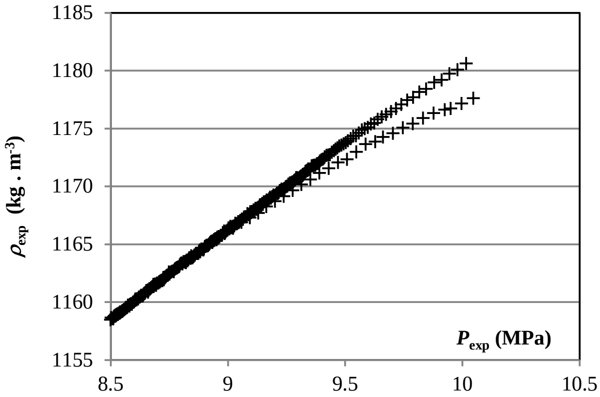

Figure 4. Density as a function of pressure at 348.2 K.

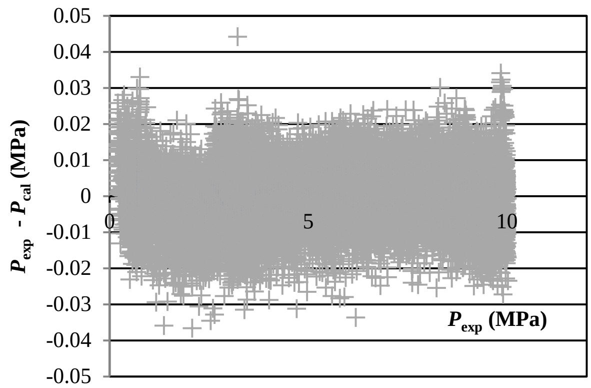

Figure 5. Deviations between experimental and calculated pressures for remaining liquid densities after consistency test treatment.

pressure sensor used. The standard deviation on the 42,240 points is 0.005 MPa, this is about ten times larger than their estimated pressure uncertainties. We can conclude uncertainties on pressures were evidently underestimated by Coquelet *et al.* [3].

Table 2 contains only the trustable data from **Tables 2**

Table 1. Densities of HFP.

Vapor densities											
T	*P*	*ρ*	*T*	*P*	*ρ*	*T*	*P*	*ρ*	*T*	*P*	*ρ*
K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$
263.41	0.1302	9.2809	263.40	0.2274	16.933	283.24	0.4445	32.350	303.28	0.7729	56.178
263.41	0.1330	9.5029	263.40	0.2294	17.053	283.24	0.4483	32.640	303.28	0.7821	57.024
263.40	0.1358	9.7287	263.41	0.2314	17.292	283.24	0.4521	32.992	303.28	0.7912	57.852
263.40	0.1386	9.9512				283.25	0.4559	33.232	303.28	0.8003	58.744
263.41	0.1415	10.136	283.23	0.2895	19.903	283.25	0.4605	33.768	303.28	0.8105	59.713
263.41	0.1442	10.379	283.24	0.2953	20.300				303.26	0.8187	60.522
263.41	0.1471	10.581	283.24	0.3035	20.988	303.28	0.4206	27.450	303.27	0.8270	61.310
263.40	0.1498	10.801	283.24	0.3084	21.365	303.27	0.4316	28.275	303.28	0.8340	62.058
263.40	0.1525	10.973	283.23	0.3133	21.707	303.28	0.4439	29.151	303.28	0.8420	62.873
263.40	0.1553	11.212	283.24	0.3174	22.036	303.28	0.4548	29.939			
263.40	0.1579	11.414	283.24	0.3222	22.368	303.28	0.4657	30.696	323.21	0.5008	30.574
263.40	0.1606	11.647	283.24	0.3270	22.770	303.28	0.4763	31.544	323.20	0.5407	33.232
263.40	0.1632	11.833	283.24	0.3312	23.117	303.28	0.4884	32.458	323.21	0.5686	35.175
263.41	0.1659	12.035	283.24	0.3352	23.372	303.28	0.5004	33.397	323.20	0.6033	37.627
263.41	0.1686	12.218	283.24	0.3400	23.845	303.27	0.5136	34.318	323.20	0.6395	40.168
263.41	0.1712	12.456	283.24	0.3442	24.108	303.28	0.5241	35.196	323.21	0.6750	42.784
263.41	0.1738	12.654	283.24	0.3482	24.411	303.28	0.5345	35.971	323.20	0.7098	45.300
263.41	0.1764	12.818	283.25	0.3531	24.764	303.26	0.5450	36.847	323.21	0.7373	47.337
263.40	0.1789	13.078	283.24	0.3571	25.072	303.27	0.5555	37.603	323.20	0.7846	50.994
263.40	0.1815	13.237	283.25	0.3611	25.445	303.28	0.5658	38.412	323.21	0.8254	54.173
263.41	0.1839	13.463	283.24	0.3659	25.853	303.28	0.5760	39.225	323.21	0.8558	56.561
263.41	0.1864	13.619	283.24	0.3700	26.146	303.28	0.5875	40.136	323.21	0.8825	58.745
263.41	0.1890	13.817	283.24	0.3747	26.552	303.28	0.5977	41.017	323.21	0.9164	61.512
263.41	0.1913	14.012	283.24	0.3787	26.899	303.28	0.6079	41.804	323.20	0.9493	64.319
263.40	0.1938	14.200	283.24	0.3828	27.236	303.28	0.6206	42.906	323.21	0.9832	67.213
263.40	0.1961	14.396	283.24	0.3867	27.563	303.27	0.6306	43.671	323.20	1.0027	69.010
263.40	0.1985	14.629	283.25	0.3907	27.782	303.26	0.6431	44.725	323.21	1.0261	71.062
263.41	0.2009	14.793	283.24	0.3946	28.179	303.26	0.6532	45.583	323.21	1.0477	72.912
263.40	0.2032	14.983	283.24	0.3987	28.482	303.27	0.6630	46.436	323.21	1.0673	74.738
263.40	0.2055	15.135	283.24	0.4034	28.816	303.28	0.6730	47.215	323.20	1.0834	76.287
263.40	0.2078	15.384	283.24	0.4074	29.204	303.28	0.6827	48.129	323.21	1.1048	78.288
263.40	0.2099	15.521	283.24	0.4114	29.532	303.28	0.6936	49.011	323.20	1.1256	80.357
263.40	0.2123	15.707	283.25	0.4162	29.928	303.27	0.7033	49.884	323.21	1.1401	81.784
263.40	0.2146	15.892	283.24	0.4209	30.373	303.27	0.7129	50.724	323.20	1.1552	83.245
263.41	0.2167	16.078	283.24	0.4248	30.649	303.28	0.7237	51.658	323.21	1.1675	84.433
263.40	0.2188	16.238	283.24	0.4287	31.045	303.28	0.7344	52.626	323.21	1.1932	87.022
263.40	0.2211	16.431	283.25	0.4327	31.286	303.28	0.7450	53.664	323.20	1.2070	88.441
263.40	0.2232	16.590	283.24	0.4366	31.702	303.27	0.7544	54.477	323.20	1.2204	89.889

263.40	0.2254	16.763	283.24	0.4405	31.968	303.27	0.7637	55.342	323.22	1.2326	91.079
T	P	ρ	T	P	ρ	T	P	ρ	T	P	ρ
K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}
323.21	1.2442	92.409	343.23	2.1308	184.26	353.13	2.7613	297.64	355.25	2.8628	314.75
323.20	1.2549	93.544	343.22	2.1433	186.60	353.13	2.7695	302.00	355.25	2.8754	322.19
323.20	1.2762	95.862	343.24	2.1553	188.96	353.13	2.7781	307.16	355.25	2.8897	331.26
323.21	1.2944	97.960	343.25	2.1668	191.26	353.13	2.7816	309.46	355.25	2.9013	340.48
323.20	1.3116	99.800	343.25	2.1791	193.71						
323.20	1.3280	101.85	343.21	2.1901	196.25	355.25	1.5818	101.98	357.02	1.6048	102.77
323.20	1.3436	103.60	343.25	2.2014	198.59	355.25	1.6143	104.74	357.02	1.6737	108.67
323.21	1.3567	105.23	343.21	2.2117	200.97	355.25	1.6455	107.51	357.01	1.7418	114.76
						355.26	1.6750	110.13	357.02	1.8085	120.92
343.24	1.5744	110.45	353.12	1.9032	134.30	355.25	1.7016	112.53	357.02	1.8630	126.06
343.24	1.5997	113.00	353.13	1.9573	140.03	355.25	1.7255	114.77	357.02	1.9167	131.37
343.25	1.6236	115.44	353.12	2.0110	146.07	355.25	1.7498	116.98	357.03	1.9716	137.03
343.23	1.6467	117.95	353.13	2.0621	152.10	355.25	1.7730	119.17	357.04	2.0258	142.64
343.24	1.6692	120.33	353.13	2.1096	157.94	355.25	1.7961	121.37	357.04	2.0760	148.19
343.25	1.6910	122.68	353.13	2.1541	163.58	355.26	1.8170	123.34	357.04	2.1232	153.54
343.25	1.7127	125.08	353.13	2.1957	169.10	355.25	1.8369	125.28	357.04	2.1646	158.38
343.25	1.7340	127.50	353.13	2.2439	175.75	355.25	1.8567	127.27	357.04	2.2085	163.72
343.25	1.7549	129.82	353.13	2.2824	181.43	355.25	1.9085	132.51	357.04	2.2521	169.16
343.25	1.7746	132.14	353.13	2.3162	186.58	355.26	1.9678	138.66	357.04	2.2920	174.38
343.23	1.7948	134.67	353.14	2.3510	192.05	355.26	2.0205	144.41	357.03	2.3295	179.35
343.24	1.8160	137.14	353.14	2.3839	197.48	355.25	2.0652	149.45	357.03	2.3675	184.68
343.24	1.8338	139.44	353.14	2.4158	202.92	355.25	2.1148	155.31	357.02	2.4042	190.03
343.25	1.8513	141.49	353.14	2.4435	208.12	355.25	2.1600	160.70	357.02	2.4384	195.20
343.20	1.8694	143.90	353.14	2.4703	213.14	355.24	2.2060	166.59	357.03	2.4724	200.51
343.23	1.8871	146.21	353.13	2.4969	218.39	355.24	2.2495	172.29	357.02	2.5056	206.01
343.25	1.9054	148.67	353.13	2.5216	223.60	355.24	2.2886	177.69	357.03	2.5368	211.33
343.24	1.9225	151.01	353.13	2.5455	228.69	355.24	2.3246	182.73	357.03	2.5673	216.75
343.22	1.9391	153.27	353.14	2.5669	233.65	355.24	2.3632	188.54	357.03	2.5958	221.98
343.21	1.9556	155.71	353.13	2.5871	238.54	355.24	2.4181	197.16	357.04	2.6233	227.25
343.18	1.9720	158.13	353.13	2.6065	243.48	355.24	2.4750	206.70	357.04	2.6502	232.68
343.22	1.9832	159.75	353.13	2.6241	248.17	355.24	2.5285	216.42	357.03	2.6749	237.96
343.24	1.9963	161.60	353.13	2.6411	252.95	355.24	2.5783	226.29	357.04	2.6927	241.91
343.23	2.0108	163.82	353.13	2.6582	257.83	355.24	2.6212	235.50	357.04	2.7212	248.45
343.25	2.0246	165.97	353.13	2.6734	262.52	355.24	2.6635	245.20	357.04	2.7567	257.14
343.24	2.0379	168.09	353.13	2.6872	267.15	355.24	2.6996	254.54	357.04	2.7878	265.41
343.23	2.0520	170.29	353.13	2.7007	271.80	355.25	2.7333	263.91	357.04	2.8115	272.21
343.25	2.0658	172.70	353.13	2.7134	276.52	355.24	2.7628	273.22	357.04	2.8375	280.22
343.25	2.0793	174.97	353.13	2.7249	281.02	355.24	2.7902	282.60	357.04	2.8621	288.49
343.25	2.0927	177.24	353.13	2.7342	285.02	355.24	2.8116	290.74	357.03	2.8830	296.29
343.25	2.1060	179.66	353.13	2.7444	289.45	355.24	2.8311	299.13	357.03	2.8951	301.32

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343.21	2.1185	181.99	353.12	2.7537	293.77	355.24	2.8486	307.39	357.03	2.9003	303.89
T	*P*	*ρ*	*T*	*P*	*ρ*	*T*	*P*	*ρ*	*T*	*P*	*ρ*
K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}
357.03	2.9107	308.24	358.11	2.3484	180.01	358.14	3.0297	350.44	362.88	2.5683	199.28
357.03	2.9234	313.91	358.12	2.3729	183.30	358.16	3.0785	391.31	362.88	2.6231	207.21
357.03	2.9363	320.08	358.12	2.3945	186.40				362.87	2.6736	215.10
357.03	2.9582	331.37	358.12	2.4147	189.24	362.89	1.6026	98.83	362.88	2.7182	222.25
357.03	2.9777	343.50	358.12	2.4316	191.77	362.90	1.6666	104.27	362.88	2.7545	228.42
357.05	3.0070	365.19	358.13	2.4492	194.38	362.90	1.7208	108.65	362.87	2.7843	233.81
			358.12	2.4637	196.64	362.90	1.7711	112.78	362.87	2.8064	237.98
358.10	1.6004	101.77	358.12	2.4802	199.08	362.89	1.8181	116.83	362.87	2.8272	241.92
358.10	1.6902	109.47	358.13	2.4961	201.53	362.89	1.8613	120.81	362.86	2.8487	246.13
358.10	1.7717	116.73	358.12	2.5087	203.68	362.89	1.8920	123.41	362.87	2.8840	253.16
358.10	1.8445	123.53	358.12	2.5211	205.69	362.89	1.9269	126.55	362.87	2.9014	256.91
358.11	1.9099	129.77	358.13	2.5339	207.80	362.89	1.9594	129.59	362.87	2.9269	262.44
358.10	1.9529	133.98	358.13	2.5466	209.81	362.89	1.9911	132.66	362.87	2.9783	274.33
358.11	2.0055	139.40	358.12	2.5553	211.41	362.88	2.0213	135.65	362.88	3.0746	299.37
358.11	2.0530	144.47	358.13	2.6325	225.14	362.88	2.0506	138.29	362.90	3.1534	325.03
358.11	2.0992	149.52	358.13	2.7116	241.11	362.88	2.0762	141.04	362.89	3.2150	350.25
358.10	2.1400	154.11	358.13	2.7772	256.23	362.88	2.1156	144.99	362.89	3.2634	375.24
358.10	2.1760	158.32	358.13	2.8259	269.03	362.88	2.1828	152.15	362.89	3.3028	401.16
358.10	2.2109	162.48	358.13	2.8632	279.95	362.88	2.2493	159.13	362.89	3.3321	426.48
358.11	2.2430	166.31	358.13	2.8932	289.65	362.88	2.3136	166.43	362.90	3.3554	452.56
358.11	2.2741	170.22	358.14	2.9456	308.34	362.88	2.3824	174.89	362.90	3.3735	478.83
358.11	2.2994	173.49	358.13	2.9749	320.98	362.87	2.4454	182.79	362.90	3.3855	500.09
358.11	2.3229	176.62	358.13	2.9952	330.70	362.88	2.5108	191.35			

Liquid and supercritical densities

T	*P*	*ρ*	*T*	*P*	*ρ*	*T*	*P*	*ρ*	*T*	*P*	*ρ*
K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}	K	MPa	kg·m^{-3}
263.49	0.2344	1462.60	263.49	3.3443	1477.99	263.50	6.8018	1493.30	283.17	0.5712	1382.89
263.49	0.4005	1463.48	263.50	3.4480	1478.47	263.51	7.0484	1494.28	283.17	0.6658	1383.60
263.49	0.5098	1464.06	263.50	3.5897	1479.11	263.50	7.2675	1495.21	283.17	0.7214	1383.94
263.50	0.6902	1464.99	263.49	3.7777	1480.02	263.51	7.5076	1496.20	283.16	0.8365	1384.86
263.50	0.7793	1465.45	263.50	3.9414	1480.72	263.49	7.7506	1497.24	283.16	1.0396	1386.34
263.49	0.8440	1465.81	263.50	4.1241	1481.55	263.52	8.0413	1498.34	283.17	1.6324	1390.59
263.50	1.1187	1467.16	263.51	4.3378	1482.55	263.51	8.3648	1499.70	283.16	2.2501	1394.87
263.49	1.4771	1469.01	263.50	4.6165	1483.82	263.50	8.5930	1500.66	283.16	2.6648	1397.57
263.49	1.8313	1470.78	263.50	4.9541	1485.33	263.50	8.8186	1501.54	283.15	2.7118	1397.93
263.49	2.1807	1472.49	263.50	5.2620	1486.69	263.50	9.0842	1502.59	283.14	2.8054	1398.54
263.50	2.5772	1474.41	263.50	5.6047	1488.17	263.50	9.3944	1503.80	283.16	2.9493	1399.47
263.49	2.8130	1475.50	263.50	6.0257	1490.01	263.50	9.7162	1505.07	283.16	2.9927	1399.77
263.49	2.9795	1476.28	263.49	6.2416	1490.94	263.51	9.99	1506.07	283.17	2.9971	1399.77
263.49	3.1959	1477.28	263.50	6.4174	1491.65				283.17	2.9998	1399.80

263.50	3.2614	1477.57	263.50	6.5911	1492.39	283.17	0.4698	1382.04	283.17	3.0382	1400.05

T	P	ρ	T	P	ρ	T	P	ρ	T	P	ρ
K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$
283.16	3.1615	1400.87	303.37	2.7849	1309.16	323.36	3.2630	1209.83	343.18	3.2770	1072.74
283.16	3.2296	1401.33	303.36	2.9185	1310.51	323.37	3.5588	1214.48	343.14	3.4333	1078.74
283.16	3.2728	1401.61	303.36	2.9307	1310.67	323.36	3.6720	1216.27	343.15	3.5963	1084.50
283.16	3.3637	1402.20	303.38	2.9933	1311.27	323.36	3.7893	1218.14	343.10	3.8060	1091.78
283.17	3.5116	1403.13	303.37	3.0866	1312.17	323.36	3.9397	1220.38	343.10	3.9148	1095.09
283.17	3.6663	1404.11	303.38	3.1857	1313.13	323.36	4.0934	1222.65	343.10	4.0523	1099.41
283.15	3.8026	1405.02	303.37	3.2693	1313.88	323.36	4.2825	1225.41	343.15	4.1954	1103.09
283.15	3.9872	1406.17	303.37	3.3126	1314.39	323.37	4.4794	1228.20	343.15	4.3449	1107.25
283.15	4.1863	1407.41	303.37	3.4926	1316.15	323.36	4.6979	1231.27	343.08	4.4776	1111.27
283.15	4.4758	1409.19	303.37	3.7235	1318.30	323.36	4.9172	1234.22	343.13	4.6043	1114.20
283.16	4.8504	1411.46	303.37	3.9594	1320.48	323.36	5.1432	1237.21	343.14	4.7474	1117.85
283.16	5.1823	1413.45	303.36	4.2842	1323.48	323.37	5.3859	1240.33	343.13	4.8853	1121.19
283.16	5.4802	1415.20	303.37	4.7074	1327.25	323.36	5.6525	1243.74	343.14	5.0337	1124.78
283.17	5.6908	1416.42	303.37	5.1888	1331.39	323.36	5.8633	1246.31	343.16	5.1610	1127.67
283.17	5.9249	1417.79	303.37	5.5877	1334.67	323.36	6.0183	1248.17	343.11	5.2809	1130.51
283.16	6.1474	1419.06	303.36	5.7419	1335.96	323.36	6.2000	1250.33	343.15	5.4296	1133.72
283.17	6.4221	1420.61	303.38	5.9178	1337.36	323.37	6.3922	1252.57	343.13	5.5803	1136.99
283.16	6.6614	1421.98	303.37	6.0895	1338.75	323.36	6.5607	1254.59	343.13	5.7458	1140.49
283.16	6.9272	1423.44	303.36	6.2521	1340.07	323.37	6.7801	1257.08	343.09	5.9144	1144.10
283.16	7.1758	1424.82	303.37	6.4774	1341.86	323.36	7.0081	1259.57	343.13	6.1494	1148.49
283.16	7.4145	1426.14	303.37	6.7016	1343.59	323.37	7.2360	1262.04	343.15	6.3754	1152.64
283.16	7.8586	1428.50	303.36	6.9381	1345.42	323.36	7.4970	1264.90	343.12	6.6420	1157.63
283.16	8.3282	1431.01	303.37	7.2007	1347.40	323.37	7.7482	1267.53	343.12	6.9374	1162.77
283.16	8.6936	1432.92	303.37	7.4843	1349.56	323.36	8.0400	1270.52	343.16	7.1456	1166.09
283.16	9.1257	1435.16	303.37	7.7694	1351.63	323.37	8.3358	1273.49	343.13	7.3143	1169.11
283.17	9.6012	1437.53	303.37	8.0990	1354.02	323.36	8.6540	1276.62	343.15	7.5136	1172.21
283.16	10.00	1439.52	303.38	8.4005	1356.17	323.36	8.8450	1278.47	343.15	7.7097	1175.33
			303.38	8.7837	1358.84	323.36	9.0517	1280.45	343.13	7.9291	1178.74
303.36	0.85	1287.97	303.38	9.1799	1361.62	323.36	9.2694	1282.50	343.13	8.1778	1182.49
303.37	0.9378	1288.97	303.37	9.7063	1365.14	323.36	9.4714	1284.41	343.13	8.4071	1185.80
303.37	0.9511	1289.14	303.37	9.99	1367.03	323.36	9.7097	1286.55	343.10	8.6707	1189.51
303.36	1.0541	1290.38	323.37	1.42	1174.31	323.36	9.9458	1288.68	343.12	9.0310	1194.37
303.37	1.1573	1291.56	323.36	1.5746	1177.86	323.36	9.99	1289.15	343.17	9.4439	1199.72
303.36	1.2988	1293.20	323.36	1.7619	1181.93				343.07	9.8832	1205.55
303.37	1.4773	1295.32	323.36	1.9856	1186.54	343.11	2.38	1030.41	343.13	9.9823	1206.55
303.36	1.6090	1296.75	323.37	2.1895	1190.59	343.18	2.5875	1041.95			
303.36	1.8082	1298.96	323.36	2.4451	1195.49	343.18	2.7999	1052.25	348.15	2.5063	959.57
303.36	1.9951	1301.01	323.36	2.7330	1200.72	343.17	2.8793	1056.54	348.15	2.5807	967.62
303.37	2.2154	1303.37	323.36	2.8503	1202.76	343.17	2.9726	1060.25	348.15	2.6650	975.74
303.36	2.4610	1305.98	323.36	2.9981	1205.34	343.14	3.0434	1063.62	348.15	2.7670	984.43

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303.37	2.6970	1308.28	323.36	3.0089	1205.47	343.18	3.1646	1068.25	348.14	2.8350	989.71
T	P	ρ	T	P	ρ	T	P	ρ	T	P	ρ
K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$	K	MPa	$kg \cdot m^{-3}$
348.15	2.8998	994.57	353.10	2.9255	912.33	357.02	3.1111	833.74	362.88	3.5137	727.62
348.15	2.9771	999.82	353.12	2.9622	917.80	357.02	3.1712	852.76	362.90	3.5720	762.04
348.15	2.9924	1000.80	353.12	2.9893	921.43	357.01	3.2529	871.60	362.92	3.6667	797.39
348.13	3.0241	1003.27	353.13	2.9998	922.83	357.01	3.3072	882.00	362.92	3.7773	826.35
348.15	3.1686	1011.94	353.13	3.0507	929.65	357.02	3.3780	893.55	362.93	3.8981	849.28
348.14	3.3388	1021.49	353.10	3.1188	938.02	357.03	3.4703	906.34	362.92	3.9491	857.62
348.13	3.5586	1032.40	353.13	3.2195	948.23	357.03	3.5628	917.41	362.92	4.0139	867.25
348.14	3.6615	1037.05	353.14	3.3175	957.33	357.01	3.6121	923.16	362.92	4.0824	876.48
348.14	3.7808	1042.19	353.13	3.4302	966.82	357.00	3.6702	929.31	362.92	4.1528	885.28
348.15	3.8951	1046.96	353.13	3.5523	976.05	357.01	3.7558	937.42	362.91	4.2311	894.18
348.14	4.0246	1052.08	353.13	3.6916	985.56	357.01	3.8510	945.66	362.91	4.3262	903.88
348.13	4.1628	1057.39	353.12	3.8631	996.09	357.01	3.9570	954.08	362.91	4.4244	913.15
348.13	4.3298	1063.41	353.13	4.0712	1007.44	357.02	4.0890	963.54	362.90	4.5292	922.20
348.14	4.5222	1069.87	353.12	4.3084	1019.03	357.02	4.2311	972.86	362.89	4.6511	931.84
348.14	4.7012	1075.55	353.12	4.5492	1029.60	357.02	4.4027	983.12	362.90	4.8021	942.47
348.14	4.8352	1079.64	353.12	4.7878	1039.11	357.02	4.5908	993.37	362.92	4.9814	953.96
348.13	4.9330	1082.55	353.13	5.0040	1047.06	357.02	4.8261	1004.87	362.92	5.1603	964.26
348.13	5.0774	1086.71	353.13	5.2259	1054.73	357.02	5.0853	1016.35	362.92	5.2834	970.93
348.14	5.2077	1090.33	353.13	5.4583	1062.16	357.02	5.3577	1027.14	362.93	5.4501	979.39
348.14	5.3649	1094.65	353.13	5.6592	1068.32	357.03	5.5121	1032.88	362.92	5.5832	985.74
348.14	5.5644	1099.78	353.13	5.8803	1074.71	357.02	5.6709	1038.54	362.93	5.7812	994.50
348.13	5.7912	1105.44	353.13	6.0511	1079.42	357.02	5.8365	1044.18	362.93	5.9198	1000.30
348.14	6.0365	1111.21	353.14	6.2400	1084.40	357.02	6.0264	1050.30	362.92	6.0494	1005.54
348.13	6.3062	1117.33	353.13	6.4190	1089.01	357.02	6.1898	1055.34	362.92	6.2176	1012.03
348.14	6.6047	1123.73	353.15	6.6542	1094.70	357.00	6.3067	1058.93	362.92	6.3845	1018.10
348.13	6.8303	1128.36	353.14	6.8350	1099.00	357.02	6.4757	1063.71	362.92	6.5749	1024.73
348.12	7.0392	1132.55	353.14	7.0278	1103.39	357.01	6.6403	1068.34	362.91	6.7692	1031.15
348.12	7.2462	1136.50	353.15	7.2508	1108.26	357.02	6.8284	1073.32	362.91	6.9763	1037.63
348.12	7.4780	1140.85	353.14	7.4607	1112.69	357.02	7.0299	1078.51	362.91	7.2208	1044.90
348.11	7.7121	1145.16	353.14	7.6879	1117.39	357.01	7.2375	1083.67	362.90	7.4626	1051.74
348.12	7.9409	1149.12	353.13	7.9294	1122.16	357.02	7.4729	1089.23	362.89	7.7376	1059.06
348.12	8.1996	1153.54	353.12	8.1999	1127.34	357.01	7.7275	1095.06	362.89	8.0418	1066.74
348.12	8.4235	1157.17	353.09	8.4395	1131.92	357.01	7.9973	1100.94	362.89	8.3779	1074.76
348.12	8.6747	1161.26	353.06	8.6677	1136.08	357.01	8.2949	1107.17	362.89	8.7464	1083.00
348.13	8.9460	1165.39	353.06	9.0076	1141.95	357.02	8.6373	1113.95	362.89	8.9576	1087.48
348.14	9.2995	1170.72	353.07	9.3594	1147.74	357.02	8.9868	1120.56	362.88	9.1065	1090.63
348.16	9.95	1179.71	353.07	9.7590	1154.06	357.01	9.3930	1127.88	362.88	9.2777	1094.12
353.13	2.79	883.82	353.06	10.00	1157.73	357.02	9.8823	1136.21	362.88	9.4571	1097.66
353.12	2.8200	892.36				357.02	9.9954	1138.05	362.88	9.6459	1101.34
353.10	2.8439	897.65	357.00	3.02	777.77				362.88	9.8470	1105.11

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353.11	2.8887	906.09	357.02	3.0532	807.50	362.88	3.47	691.30	362.88	9.9964	1107.95

and 3 of original paper [3]. Other trustable data (about 10500 over the 48000 original raw data) are available from corresponding author: laugier@enscbp.fr.

4. Conclusions

Through the present study we have pointed out the importance of reliable and accurate data and the usefulness of simple data consistency tests. These simple tests justify the development of various performing techniques such as those based on neural network.

Density of gases and gas mixtures must tend to zero when pressure tends to zero and additionally the virial law must be followed.

Neural network based approach presently used to assess the quality of experimental hexafluoropropylene densities gives encouraging results.

For supercritical HFP only one isotherm has been conserved from previous work [3]. Due to high thermal effects in the vicinity of critical point, it would have been certainly necessary to be more careful and more patient recording the data (very small pressure changes are requested as a function of time).

Finally, we conclude neural network modeling is worth in the assessment of data consistency.

As far as high pressure vibrating tube densimeters are used, vapor densities at very low pressures are better determined through extrapolation of higher pressure values using virial equation of state.

Only trustable densities for the three vapor, liquid and supercritical physical states have been reported herein.

Supporting Information Available:

Density values of HFP at various temperatures and in its various states: vapor, liquid and supercritical. This material is available upon demand to corresponding author: laugier@enscbp.fr. It has to be used preferably to the material presented in Coquelet *et al.*'s paper [3] that unfortunately contains inaccurate and erroneous data.

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